

Two-mode variational Monte Carlo study of Quasiparticle excitations in cuprates

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Recent measurements of quasiparticles in hole-doped cuprates reveal highly unusual features: 1) the doping-independent Fermi velocity, 2) two energy scales in the quasiparticle spectral function, and 3) a suppression of the low energy spectral weight near the zone center. The underlying mechanism is under hot debate. We addressed these important issues by a novel two-mode variational Monte Carlo (VMC) study of the t-J model. We obtained results in agreement with the experiments but without invoking extrinsic effects. Besides, we resolved a long standing issue of the sum rule for quasiparticle spectral weights in VMC studies. The electron doped case was also discussed.

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Understanding the quasiparticle excitations is a prelude to unravel the mechanism of high-Tc superconductivity. Recent angle-resolved photo-emission spectra (ARPES) in cuprates reveal highly unusual features and lead to hot debates. For example, on the low energy quasiparticle band the nodal Fermi velocity does not seem to increase with increasing doping, and is called a "universal nodal Fermi velocity".[1] This seems to challenge the concept of doped Mott insulators which would naively predict a vanishing Fermi velocity with decreasing doping. On the other hand, ARPES measurements up to higher energies [2–9] revealed that the quasi-particle dispersion along the nodal direction breaks up near the momentum $(\pi/4, \pi/4)$ at an energy around 0.3 ~ 0.4 eV (or the low energy spectral weight near the Γ seems to disappear), and reappeared around 1eV. The two bands are connected in a waterfall fashion in the momentum-energy space. This high energy anomaly has intrigued many theoretical studies and disputes.[2, 10–17] A central concern is whether the anomaly is caused by extrinsic effects due to phonons, or is an intrinsic property of the strongly correlated electrons themselves. We summarize the main important issues that will concern us in this Letter: 1) the doping-independent Fermi velocity, 2) two energy scales in the quasiparticle spectral function, and 3) a suppression of the low energy spectral weight near the zone center.

We address the above important issues within the commonly accepted one-band t-J model without invoking other extrinsic effects. The theoretical machinery we use is the Gutzwiller projection variational Monte Carlo (VMC). It proves to give good energy and supports d-wave pairing symmetry.[18–22] As for quasiparticle excitations under concern, a projected mean-field excited state is commonly used in the literature.[23–25] For a given momentum \mathbf{k} and spin σ , only one such quasiparticle can be constructed. We call such an approach as a single-mode approach (SMA). Unfortunately, the SMA gives only a single low energy band and predicts that the spectral weight is maximal at the center of the Brillouine zone (the Γ point), in contrast to the two energy scales and suppression of low energy spectral weight re-

vealed by ARPES. The spectral weight below the Fermi level captured by SMA is proved to be smaller than the exact value $1 - x$. [23, 26] It is therefore likely that the high energy feature is due to the missing spectral weight beyond the SMA. Moreover, the nodal Fermi velocity increases significantly with doping in such an approach.[25] In this Letter we design a two-mode approach (TMA) for each set of quasiparticle quantum number (\mathbf{k}, σ) . We show that the TMA satisfies the spectral sum rules for quasiparticle excitations both below and above the Fermi level, resolving a long standing problem SMA.[27] In this way spectral weights beyond the scope of the SMA can also be captured. Our numerical results are in agreement with the main experimental features listed above. We also demonstrate that in the electron doped case there should be no high energy anomaly below the Fermi level, in agreement with the finite temperature exact diagonalization.[14]

The t-J model Hamiltonian is $H = H_t + H_J$, with $H_t = -\sum_{\langle ij \rangle, \sigma} t_{ij} (P_G c_{i\sigma}^\dagger c_{j, \sigma} P_G + \text{h.c.})$ and $H_J = J \sum_{\langle ij \rangle} (S_i \cdot S_j - \frac{1}{4} P_G n_i n_j P_G)$. [28] Here $t_{ij} = t_1, t_2, t_3$ are hopping integral between the nearest, second-nearest and third-nearest neighbor sites i and j , $c_{i\sigma}$ is the electron annihilation operator, S_i is the electron spin, $n_i = n_{i\uparrow} + n_{i\downarrow}$ with $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $P_G = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$ is the Gutzwiller projection operator that removes any double occupations. A widely used trial ground state with d-wave pairing is $|\Psi_{GS}\rangle = P_G P_N |\Psi_{dBCS}\rangle$, [18] where P_N is the projection operator that fixes the number of electrons, $|\Psi_{dBCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle$. Here $u_{\mathbf{k}}^2 = \frac{1}{2}(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}})$, $v_{\mathbf{k}}^2 = \frac{1}{2}(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}})$, $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$, $\xi_{\mathbf{k}} = -2(\cos k_x + \cos k_y) - 4t'_{var} \cos k_x \cos k_y - 2t''_{var}(\cos 2k_x + \cos 2k_y) - \mu_{var}$, $\Delta_{\mathbf{k}} = \Delta_{var}(\cos k_x - \cos k_y)$. t'_{var} , t''_{var} , Δ_{var} and μ_{var} are variational parameters. In the following we concentrate on the quasiparticle excitations. Candidates for such excitations are described by the quasi-hole, bare-hole, quasi-electron and bare-electron wave

functions as follows:

$$|\Psi_{qh}(k, \sigma)\rangle = P_G P_{N-1} \gamma_{k\sigma}^\dagger |\Psi_{dBCS}\rangle, \quad (1)$$

$$|\Psi_{bh}(k, \sigma)\rangle = c_{-k, -\sigma} |\Psi_{GS}\rangle, \quad (2)$$

$$|\Psi_{qe}(k, \sigma)\rangle = P_G P_{N+1} \gamma_{k\sigma}^\dagger |\Psi_{dBCS}\rangle, \quad (3)$$

$$|\Psi_{be}(k, \sigma)\rangle = c_{k, \sigma}^\dagger |\Psi_{GS}\rangle. \quad (4)$$

Here $\gamma_{k\sigma} = u_k c_{k\sigma} - \sigma v_k c_{-k\bar{\sigma}}^\dagger$ is the Bogoliubov quasi-particle annihilation operator with momentum k and spin σ . As pointed out by Ran et al, all these wave functions on for a specific real-space electron configuration can be written in the form of determinants.[29] Thus the overlaps between these states can be computed statistically. To ease further discussion we denote the normalized wave functions for the ground state, the quasi-hole, the bare-hole, the quasi-electron and the bare-electron states as, respectively, $|GS\rangle$, $|QH\rangle$, $|BH\rangle$, $|QE\rangle$ and $|BE\rangle$. The subscripts k and σ are left implicit.

The ARPES experiment measures the one particle spectral function $A(k, \omega)$ in the occupied side ($\omega < 0$). According to the Lehmann representation,

$$A(k, \omega) = \sum_{n, \sigma} [|\langle n | c_{k\sigma}^\dagger | 0 \rangle|^2 \delta(\omega + \omega_0 - \omega_n) + |\langle n | c_{-k, -\sigma} | 0 \rangle|^2 \delta(\omega - \omega_0 + \omega_n)]. \quad (5)$$

Here $|n\rangle$ denotes an excited eigenstate of $H - \mu N$ with the eigenvalue ω_n . We define $Z_n^- = |\langle n | c_{k\sigma} | 0 \rangle|^2$ and $Z_n^+ = |\langle n | c_{k\sigma}^\dagger | 0 \rangle|^2$ as the spectral weights of $|n\rangle$ in the occupied and unoccupied sides, respectively. For a free particle system, the state with the quantum numbers (\mathbf{k}, σ) is unique. This is no longer the case in an interacting system. We recall that $|QH\rangle$ is the only state used in SMA. As mentioned above, the spectral weights not captured by SMA are likely to appear at higher energies, and this motivates us to go beyond the SMA by enforcing the sum rule.

In principle one should construct a complete set of excitations to satisfy the sum rule. This is possible by exact diagonalization but is limited by the lattice size. We therefore take a simpler route but still keep the sum rule. The idea is as follows. Since $[c_{k\sigma}, P_G] \neq 0$, $|QH\rangle$ and $|BH\rangle$ are neither identical nor orthogonal. We can reconstruct two orthogonal states $|BH\rangle$ and $|\eta\rangle = \frac{1}{\sqrt{1-\kappa^2}}(|QH\rangle - \kappa|BH\rangle)$ for each set of quantum numbers (\mathbf{k}, σ) , where $\kappa = \langle BH | QH \rangle$. The Hamiltonian matrix in this basis space is

$$(H)_{2 \times 2} = \begin{pmatrix} \langle \eta | H | \eta \rangle & \langle \eta | H | BH \rangle \\ \langle BH | H | \eta \rangle & \langle BH | H | BH \rangle \end{pmatrix}, \quad (6)$$

which we diagonalize to get the eigenstates $|1\rangle$ and $|2\rangle$ as linear combinations of $|BH\rangle$ and $|\eta\rangle$ (and thus of $|BH\rangle$ and $|QH\rangle$). The occupied spectral weight for (\mathbf{k}, σ) is now

given by

$$\begin{aligned} & Z_{k\sigma,1}^- + Z_{k\sigma,2}^- \\ &= \frac{|\langle 1 | c_{-k, -\sigma} | \Psi_{GS} \rangle|^2}{\langle \Psi_{GS} | \Psi_{GS} \rangle} + \frac{|\langle 2 | c_{-k, -\sigma} | \Psi_{GS} \rangle|^2}{\langle \Psi_{GS} | \Psi_{GS} \rangle} \\ &= \frac{\langle \Psi_{bh} | (|1\rangle\langle 1| + |2\rangle\langle 2|) | \Psi_{bh} \rangle}{\langle \Psi_{bh} | \Psi_{bh} \rangle} \frac{\langle \Psi_{bh} | \Psi_{bh} \rangle}{\langle \Psi_{GS} | \Psi_{GS} \rangle} \\ &= \frac{\langle \Psi_{bh} | \Psi_{bh} \rangle}{\langle \Psi_{GS} | \Psi_{GS} \rangle} = n_{-k, -\sigma}, \end{aligned} \quad (7)$$

where we used definition of the unnormalized bare-hole state. We also used the crucial fact that $|\Psi_{bh}\rangle$ lies within the space spanned by $|1\rangle$ and $|2\rangle$, or equivalently by $|BH\rangle$ and $|\eta\rangle$. By summing over (\mathbf{k}, σ) we get a total occupied spectral weight $\sum_{k\sigma} n_{k\sigma} / S = 1 - x$, with S the number of lattice size, as required by the sum rule.[26] We call the above procedure as a two-mode approach (TMA) for the excitations in the occupied side (or below the Fermi level). On the unoccupied side, since $P_G[c^\dagger, P_G] = 0$ the bare-electron and quasi-electron states are identical within the Hilbert space of the model, and one can prove that the total spectral weight of $|QE\rangle$ already satisfies the sum rule $\sum_{k\sigma} Z_{k\sigma}^+ / S = 2x$. [25, 26]

We perform Monte Carlo calculations for the energy and spectral weight of the states $|1\rangle$ and $|2\rangle$ below the Fermi level, and of the state $|QE\rangle$ above the Fermi level. We also present the results under SMA for comparison. The calculation is done on a 10×10 lattice. Larger sizes up to 14×14 are also attempted which do not alter the conclusions we reach. In our calculation we use 200,000 samples to reduce the statistical error, which we find to be less than 5 meV for quasiparticle energies. In order to get finer resolution in momentum space we use four combinations of periodic and anti-periodic boundary conditions. It turns out that the quasi-hole and quasi-electron bands are symmetric in energy,[25] and we define the central energy as the Fermi level. In Figs.1, the linear size of the symbols represents the momentum-dependent spectral weight, while the central position of the symbols represent the quasi-particle energy as a function of momentum along the cuts $(0, 0) \rightarrow (\pi, \pi) \rightarrow (\pi, 0) \rightarrow (0, 0)$. The doping levels are $x = 6\%$ (a), $x = 20\%$ (b), and $x = 30\%$ (c). The filled-blue circles are for excitations on the unoccupied side, which are identical under both SMA and TMA. The open-green circles corresponds to the result given by the SMA, which yields a single band below the Fermi level with the largest spectral weight at the Γ -point. This is a common result under SMA,[23, 24] but is inconsistent with the recent ARPES measurements. This should be contrast to the following TMA results. The filled-red and filled-pink circles are for excitations on the occupied side contributed by the lower energy eigenstate $|1\rangle$ and higher energy eigenstate $|2\rangle$, respectively. We find that along the nodal direction the spectral weight of $|1\rangle$ state at the Γ point is greatly suppressed and gradually increases away from the Γ point in the

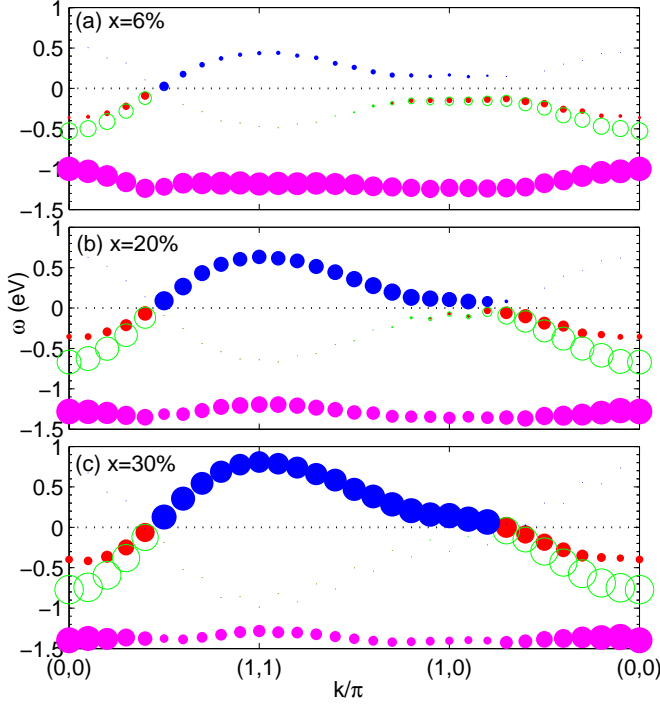


FIG. 1: (Color online) Energy dispersion and spectral weight map in the energy-momentum space (along high symmetry cuts). Only nearest hopping is included in the kinetic part of the Hamiltonian. The doping level is (a) $x = 6\%$, (b) $x = 20\%$, (c) $x = 30\%$. The spectral weight scales as linear size of the symbols. The open (filled) circles are results of SMA (TMA). The filled-blue, filled-red and filled-pink symbols denote results for quasi-electron states, 1-band from states $|1\rangle$ and 2-band from states $|2\rangle$, respectively.

nodal direction and antinodal directions. For instance, in Fig.1(a) $Z_1^-(k=0) = 0.06$ while $Z_1^-(k \sim k_F) = 0.16$. The band width below the Fermi level is roughly $0.4eV$. In the mean time, we also get a band at higher binding energy ($1.2 \sim 1.5 eV$) contributed by the states $|2\rangle$. The suppression of low energy spectral weight near the zone center and the appearance of a higher energy band are exactly what ARPES reveals. Moreover, the energy scale of the higher energy band is of order $3t$ rather than the Mott Hubbard gap (which would be infinite in a t - J model), it therefore reflects the information of soft lower Hubbard band.[13]

By inspecting Figs.1 we see that with increasing doping the spectral weight near (below or above) the Fermi level increases, while it decreases on the high energy band below the Fermi level. This signifies a gradual transfer of the spectral weight from the high energy band to the low energy bands. On the other hand, the slope of the dispersion near the nodal Fermi point barely changes for the 1-band under our TMA. The ratio among the Fermi velocities we estimated is $1 : 1.05 : 1.25$ for $x = 6\%$, 20% and 30% . This is rather consistent with the "universal

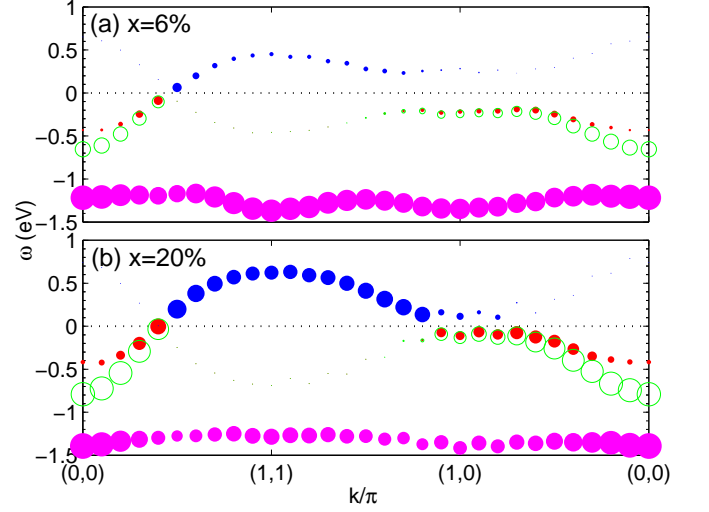


FIG. 2: (Color online) The same plot as Fig.1(a) except that a third nearest neighbor hopping is added in the Hamiltonian.

sal Fermi velocity" observed by ARPES. (Due to poor screening in cuprates, long-range Coulomb interaction at lower doping levels may have caused a slightly larger Fermi velocity on top of the correlation effects under discussion.) In contrast, the SMA (open-green symbols) gives a corresponding ratio $1 : 1.26 : 1.52$, [25] and would change more significantly in the renormalized mean field theory, [30, 31] which is rather far from the experimental result. We notice that the universal Fermi velocity was also achieved in the literature by tuning J/t [25] or by including a three-site hopping term in the Hamiltonian. [20] Finally we observe from Figs.1 that in the range of doping levels we studied, the energy scales for the low and high energy bands below the Fermi level does not change significantly. This is in agreement with the experimental results. [3, 5]

It turns out that the suppression of the low energy spectral weight near the zone center can be made more complete by including the third nearest neighbor hopping integral t_3 in the Hamiltonian and the trial wave function. For doping level $x = 6\%$, $t_1 = 0.4eV$, $t_3 = 0.06eV$ and $J = 0.12eV$ the optimal variational parameter in the trial wave function is $t'_{var} = 0.12$, $\Delta_{var} = 0.55$, $\mu_{var} = -0.28$. The quasiparticle spectra are plot in Fig.2(a). In this case $Z_1^-(k=0) = 0.045$ and $Z_1^-(k \sim k_F) = 0.18$. The curvature of the high energy dispersion near the zone center is changed as compared to the case in Fig.1(a). Similar tendency is found in Fig.2(b) as compared to Fig.1(b). We observe that the curvature also varies by inspecting published data for different families of cuprates. [2, 3, 5] We also notice that a negative second nearest neighbor hopping integral t_2 can lead to a less prominent suppression of the spectral weight near the zone center, but the existence of a higher energy band is robust.

We have also investigated the quasiparticle excitations

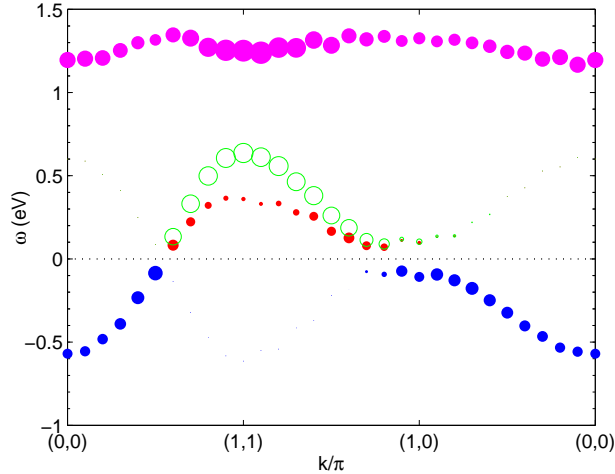


FIG. 3: (Color online) Energy dispersion and spectral weight map in the energy-momentum space (along high symmetry cuts) in an electron doped case with $x = 16\%$. Open (filled) symbols show results of SMA (TMA). The filled-blue, filled-red and filled-pink symbols denote results for quasi-hole states, 1-band from states $|1\rangle$ and 2-band from states $|2\rangle$ (in the electron picture), respectively. Notice that the high energy anomaly now appears above the Fermi level.

in electron doped cuprates, which is still described by $t - J$ models after a particle-hole transformation. We choose a doping level $x = 16\%$, at which it is believed that antiferromagnetic order does not exist. The parameters in the Hamiltonian are $t_1 = -0.4\text{eV}$ and $J = 0.12\text{eV}$. The variational parameter are the nearest neighbor singlet gap function Δ_{var} with d -wave pairing symmetry and the chemical potential μ_{var} . The optimal parameters we found are $\Delta_{var} = 0.27$ and $\mu_{var} = -0.3$. In order to relate to the results in ARPES experiments one need to switch back to the electron picture. Our result is shown in Fig.3. The filled circles are the results under TMA, and the open circles are from SMA. We find that in the electron-doped case the quasiparticle excitations below the Fermi level exhibit neither suppression of spectral weight at the zone center nor a higher energy band. This is consistent with the results of exact diagonalization.[14] Instead, a high energy band does appear but above the Fermi level. In fact, apart from some change of parameters in the Hamiltonian, the electron-doped dispersion and the associated spectral weight can be regarded as those of the hole-doped case but viewed up-side-down.

To conclude, we proposed a two-mode approach to enforce the sum rules for quasiparticle excitations both below and above the Fermi level in our Gutzwiller projection variational Monte Carlo study of doped Mott insulators described by the one-band t - J model. The TMA resolves a long standing issue regarding the sum rule in VMC.[27] In the hole doped case, we obtained results in agreement with the highly unusual features revealed

in recent angle-resolved photoemission spectra: 1) an almost doping-independent Fermi velocity, 2) two energy scales below the Fermi level, and 3) suppression of the spectral weight near the zone center on the low energy band below the Fermi level. In the electron doped case we predicted that the dispersion below the Fermi level does not have high energy anomalies.

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